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The Status of the EPA Laboratory Automation Project

Environmental Monitoring and Support Lab, Cincinnati, Ohio

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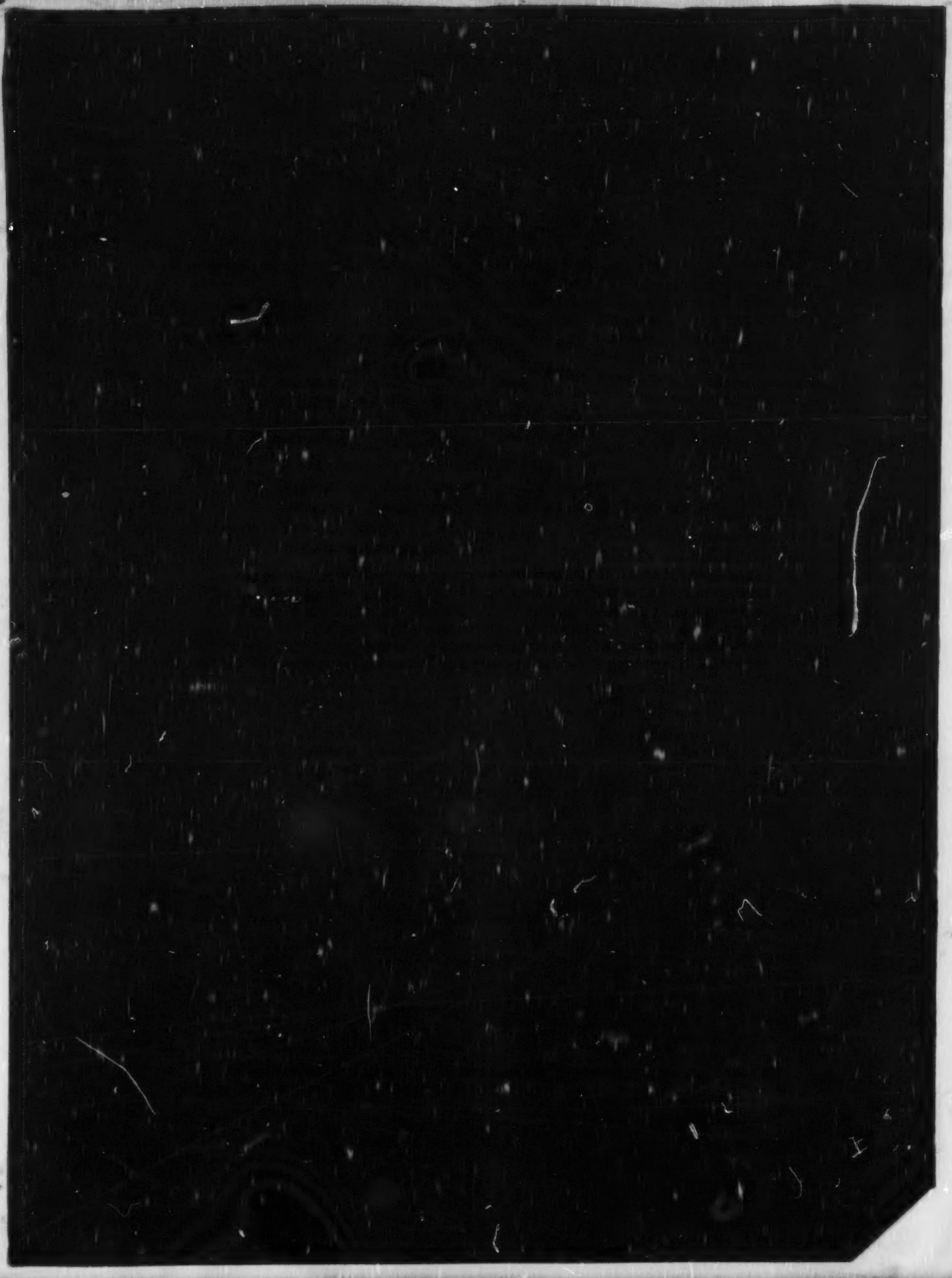

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THE STATUS OF THE EPA LABORATORY AUTOMATION PROJECT

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FOREWORD

Environmental measurements are required to determine the quality of ambient waters and the character of waste effluents. The Environmental Monitoring and Support Laboratory-Cincinnati conducts research to:

- Develop and evaluate techniques to measure the presence and concentration of physical, chemical, and radiological pollutants in water, wastewater, bottom sediments, and solid waste.
- Investigate methods for the concentration, recovery, and identification of viruses, bacteria and other microbiological organisms in water; and to determine the responses of aquatic organisms to water quality.
- Develop and operate an Agency-wide quality assurance program to assure standardization and quality control of systems for monitoring water and wastewater.

This report on the status of the EPA laboratory automation project was developed by the staff of the Physical and Chemical Methods Branch, EMSL, with the cooperation of personnel from the Cincinnati Computer Services and Systems Division, Office of Administration. It describes the status of the project as of March 1, 1977 and includes an outline of plans for future work during fiscal years 1977 and 1978. This effort has been supported by the Office of Research and Development and the Office of Planning and Management, U.S. Environmental Protection Agency, Washington, DC 20460.

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ABSTRACT

The status of the Environmental Protection Agency's laboratory automation project is described in terms of currently installed systems, and work in progress to develop and improve the system. The status report includes a management review of the project goals, a management implementation plan, and a review of the quality control aspects of laboratory automation.

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SECTION I

INTRODUCTION

The purpose of this report is to describe the current status of the Environmental Protection Agency's laboratory automation project. The first phase of this project began in January of 1973 and was concluded in June of 1974. During this period feasibility studies were completed, detailed specifications for instrument automation were written, an implementation design was developed, and a contract was let for purchase of the commercial computer hardware and the manufacturer's operating system and programming language software. Some progress in refining designs was made during the subsequent months, but the implementation phase actually began after delivery of the computer hardware in December of 1974.

At the present time three systems are installed and several studies are in progress to determine the feasibility of installing additional systems based on similar hardware and software. Each of the following sections of this report emphasizes and reviews different aspects of the project and each was intended to stand alone for readers with different interests and viewpoints. Readers' comments on any or all of these aspects are solicited and will be considered as input to subsequent status reports.

SECTION II

A MANAGEMENT OVERVIEW OF THE GENERAL GOALS OF THE PROJECT AND A MANAGEMENT IMPLEMENTATION PLAN

Before 1965 it was unthinkable to put an electronic digital computer in an analytical chemistry laboratory. Since that time the steady decreases in the cost of computers and increases in their reliability have brought about a revolution in analytical chemistry. Digital computers that were once in the $100,000 to $1,000,000 class now sell for $500 to $100,000 and have far more computational power. The analytical chemical instrumentation that has all but completely replaced the buret and filter paper is rapidly becoming computerized instrumentation.

Why is the digital computer invading the laboratory? As our technology and society have become more complex the demand for more chemical analyses in many fields has increased exponentially. Along with this increased demand there are the requirements for more accuracy, better precision, higher sensitivity, more timely results, greater selectivity, and of course all of these at a lower cost per analysis. A good example of this is the health field. At one time the family physician's stethoscope was one of the few routinely used diagnostic tools. Today a large clinical lab must do literally thousands of blood cholesterol and urine sugar analyses every day.

In the environmental field the measurement of specific air and water pollutant chemicals is the basis for the whole environmental movement. Until reliable measurements were made and correlated with undesirable health or ecological effects, environmental concern was mostly limited to those concerned with purely aesthetic values. Currently there is considerable emphasis on setting standards for acceptable air and water, issuing permits for discharge of wastes into rivers and oceans, monitoring these effluents to insure compliance with permit limitations, and conducting enforcement actions when violations occur. All of these activities are increasing the demand for more and better chemical analyses. Better analyses embodies the ideas of accuracy and precision and requires extensive use of analytical quality control techniques. Quality control is often deleted in analytical laboratories because of its cost and time requirement. With this the validity of the measurements decreases substantially. Another aspect of better analyses is the desire for new kinds of measurements that are more revealing of the state of environmental pollution than traditional measurements. These more revealing measurements are often more complex and simply cannot be accomplished economically or at all without on-line computerization.

In response to these needs in EPA, a project was started in late 1972 to develop laboratory automation methods for analytical instruments that were

owned by EPA laboratories and widely used in many monitoring and research applications. The project was a joint effort of the organizational predecessor of the Environmental Monitoring and Support Laboratory (EMSL)-Cincinnati and the Cincinnati Computer Services and Systems Division of the Office of Planning and Management (OPM). The Lawrence Livermore Laboratory of the Atomic Energy Commission (now Energy Research and Development Administration) was retained as an expert consultant in systems design and development. The goals to be achieved by laboratory automation were as follows:

(1) Improved throughput or productivity, i.e., increased sample processing capacity and the production of more timely results at a lower unit cost without the need for more personnel and instruments;

(2) Improved analytical quality control;

(3) The cost-effective measurement of more meaningful parameters; and

(4) Improved management of information about samples in process in the laboratory.

In addition to these results oriented goals, the system to be developed was required to possess the following characteristics:

(1) Applicability. The EPA laboratory automation system was intended to be applicable to a wide variety of multimedia environmental monitoring and assessment problems. Some previously developed systems were intended for very limited or specialized application.

(2) Flexibility. The EPA laboratory automation system was intended for easy modification by virtue of modular, easily duplicatable hardware and major software elements written in readily understandable, self documenting high level languages. Some other systems are literally hard wired in that it is either impossible or very costly to modify their hardware and software. The flexible, open ended design permits the continuous updating of the system with additional instruments and allows application in methods development research as well as the production atmosphere. Automation in a methods research laboratory makes possible careful testing of new procedures by allowing independent variation of a large number of method variables with a statistically significant number of test samples.

(3) Transportability. The EPA laboratory automation system was intended for easy duplication and installation in many EPA laboratories. In particular the designs for hardware interfaces between the instruments and the computer and the EPA developed software are in the public domain and may be used in any EPA laboratory without further cost. Therefore the technology is available to other EPA laboratories at a very significant cost

and time savings. Some other systems either have proprietary components or other aspects that preclude ready duplication. The transportable items are described in more detail as follows:

(a) Instrument interface hardware designs; reproduction of hardware requires funding, however, production costs are only a fraction of design costs.

(b) A group of modular assembly language programs that are written in Data General Nova assembly language. These programs are assembled into relocatable binary files that are loaded into foreground memory with the relocatable binaries of the Basic language. They are the real time data handlers, i.e., they control the acquisition of data from instruments. Since this programming is at the systems level, it is relatively complex, and all installations will use exactly the same programs. Selections of programs from the group will depend on the particular instruments automated in the laboratory.

(c) Several relatively modest modifications to the Basic language program purchased from the Data General Corporation. These modifications were necessary to incorporate the real time data handlers. These developments are at the systems level and all installations will use exactly the same program.

(d) A large group (over 25) of modular Basic language applications programs. These may be transferred directly without modification, or where necessary, modules may be modified easily to fit the operational procedures of the particular laboratory. Again the selection of programs from the group will depend on the particular instruments automated in the laboratory.

(e) All documentation for all of the above. This consists of user manuals, commented source listings, flow charts, and engineering drawings.

(4) Cost-effectiveness. The EPA laboratory automation system was intended for true cost-effectiveness with special emphasis on the above three characteristics. A major cost-effectiveness factor is the relative ease of support, maintenance, and documentation of a number of similar systems. Some other systems are relatively less cost-effective.

(5) Emphasis on Quality Control. The EPA laboratory automation system was intended to emphasize the integration of analytical quality control concepts.

In the process of designing and implementing computer systems with the

characteristics discussed above it has become well established that the top-down approach is required. This approach was employed in the EPA laboratory automation project and consists of the following sequence of events:

(1) Development of system functional specifications.

(2) Rigorous definition of all data elements.

(3) Development of a system implementation design including user interface specifications.

(4) Writing of program code concurrent with documentation.

(5) Installation, testing, and debugging of code followed by user training.

(6) Post delivery maintenance.

Most individuals not experienced in computer systems are surprised to discover that the majority of development costs for the systems that contain the above characteristics are incurred in the rigorous specifications, data definitions, and design phases of the project. With these designs in place, program coding is a straightforward, non-experimental activity. Systems conscientiously designed in such a manner also tend to be easy to install, accept, and maintain.

MANAGEMENT IMPLEMENTATION PLAN

In order to facilitate the transfer of laboratory automation technology to other EPA laboratories, a management plan was proposed. This plan is presented in terms of Functional Responsibilities and Definitions of Tasks.

Functional Responsibilities

The following functional responsibilities are consistent with Agency responsibilities:

The Office of Monitoring and Technical Support, Office of Research and Development, has responsibility for budget preparation and review, coordination with OPM and other Headquarters entities, and advocacy and support at laboratory automation policy and planning meetings.

The Management Information and Data Systems Division (MIDSD) of the Office of Planning and Management has responsibility for coordination, control, funding and approval of studies to determine the feasibility of transporting the laboratory automation system to other EPA laboratories. In addition MIDSD will approve procurements of commercially available computer hardware and software.

The Environmental Monitoring and Support Laboratory-Cincinnati has overall responsibility for the implementation of laboratory automation systems, the continued development of the system, and the long term support of the

system. This includes the funding to assemble and rigorously test systems, install systems, train EPA personnel, and provide complete documentation. These functions will be accomplished in close cooperation with CSSD and MIDSD.

The Computer Services and Systems Division-Cincinrati (CSSD) has responsibility for providing Agency-wide laboratory automation computer systems software support. The CSSD will be the focal point for the distribution, coordination, and installation of licensed, vendor's supplied systems software and modifications. Included in this is software related technical assistance and training.

The laboratory being automated has the responsibility to provide sound, realistic technical information to those who are directly responsible for the system implementation. This information consists of current and projected sample loads, operational procedures, personnel availabilities, and other information necessary to define the functional specifications. The laboratory being automated has responsibility to pay for all hardware and the commercially available components of the software. The full costs of these will be itemized in detail in the feasibility study along with the costs of possible alternatives.

After the purchase of a computer, the laboratory must provide for the maintenance of the system. The feasibility study will also detail the annual maintenance costs and include a description of personnel requirements to maintain the system and assist other personnel in its operation and use. Finally the laboratory personnel have the responsibility to refrain from modifications to software at the systems level. Systems level modifications will be supported from Cincinnati.

All laboratories interested in adopting the system will be considered for feasibility studies. The results of the Office of Research and Development laboratory evaluations will be considered if it is necessary to set priorities for feasibility studies. No system will be installed without an MIDSD approved feasibility study. Currently there exists an interagency agreement between EPA and ERDA to provide the services of the staff of the Lawrence Livermore Laboratory (LLL) for continued development and support of the laboratory automation system. This agreement covers the period from July 1, 1975 through June 30, 1980. The agreement is funded each fiscal year at a level appropriate for the projects selected for work that year.

In general no instrument type will be included in an implementation until the interface design and software have been developed, debugged, tested, and documented by EMSL-Cincinnati, usually in cooperation with Lawrence Livermore Laboratory. EMSL-Cincinnati has a long term commitment to extend laboratory automation methods to many other instruments.

An Agency-wide laboratory automation advisory committee will be formed to provide periodic input of ideas and comment. This committee will meet at least once a year to informally exchange views and technical information. The chair of the committee will be the EPA project officer for the interagency agreement. Headquarters coordination will be accomplished through the Office of Research and Development's automated data processing coordinator.

Definitions of Tasks

Each system implementation requires the completion of eleven distinct tasks that are organized into six major milestones. This section contains a description of these tasks.

Feasibility Study

1. A feasibility study and cost/benefit analysis is prepared to determine whether technology developed in previous years and currently installed in EPA monitoring laboratories should be applied to an additional EPA laboratory at a different site. Completion of this study is a major milestone, allowing management to decide to commit funds for the next phase.

Functional Specifications

2. A standard package of functional specifications and designs is modified to fit the particular laboratory. After this milestone it is possible to make valid estimates of the remaining cost to completion. Management can then, on the basis of firm costs, decide to commit funds for the completion of the project. Not until completion of the functional specifications is it possible to define the cost of automation, and management should keep open the option of discontinuing or postponing the project.

Implementation

3. A specific implementation design is prepared for each project to carry out the goals and objectives specified by Tasks 1 and 2. Designs will be based on prior designs, thereby obtaining important engineering economies.

4. Purchase specifications are prepared for the items defined by Task 3.

5. New programs are written as needed to carry out the automation, data collection, data reduction, and sample file control. Again, in the interest of standardization and economy, these will be based on programs from prior implementations. Insofar as possible, programs will be directly transferred without modification.

6. Special interfaces and other hardware needed to carry out the project are fabricated.

7. The hardware and software subsystems are assembled, tested, and debugged. Completion of this group of tasks is the third milestone.

Installation

8. Equipment is shipped to the user site, reassembled, connected to laboratory instruments, and proper operation of the complete system is verified.

9. Selected users are trained to complete the debugging process. Complete documentation of hardware and software, including user's manuals and maintenance instructions, circuit descriptions, etc. are provided. This will complete the fourth milestone.

System Evaluation

10. The installed system is evaluated against the goals, objectives, and specifications. This will include: a comparison of specified to achieved design objectives, an evaluation of user reaction to the system and its documentation based on observation and interviews, and evaluation of potential extensions to the installed system, a cost breakdown of the actual implementation, and a detailed evaluation of the benefits actually realized in increased sample throughput, enhanced precision, improved quality control, and savings in manpower.

User Assistance

11. Users are assisted in maintaining interfaces and programs and in writing software for special needs. It is likely that proprosals for new projects will be forthcoming from this work.

SECTION III

REVIEW OF THE QUALITY CONTROL ASPECTS OF LABORATORY AUTOMATION

Most users of laboratory data tend to assume that it is always of the highest quality and therefore beyond dispute. After all, analytical chemists are thoroughly professional and invariably exhibit the highest possible integrity and competence. They are highly motivated, aggressive to adopt the very latest methods, and can be trusted to put forward their very best at all times. While these points are certainly well taken, the fact remains that analytical chemists are also human beings, operating with often limited resources, and frequently under pressure to get the results out. Therefore, significant errors will and do occur and erroneous results could have a major impact on important environmental or economic decisions. Clearly the problem is one of quality control, that is, maintaining high standards for the laboratory measurements.

A closely related problem is that no measurement is perfectly exact and without some uncertainty. No matter how high the standards for the laboratory, this uncertainty will persist to a greater or lesser degree. Therefore every environmental measurement recorded should be accompanied by a realistic estimate of this error. The information required to develop this estimate can be obtained from the quality control program of the laboratory.

In a manufacturing plant quality is rarely maintained by careful inspection and rigorous testing of each and every item that comes off the assembly line. That would be too expensive! What is usually applied is a periodic, regular or sometimes random, sampling of the product. This sample is inspected and/or tested more completely than the balance of production, and overall quality control is established on a statistical basis. Periodic inspection also adds to the cost of a product, but most reputable manufacturers feel the cost is worth it.

The application of manufacturing quality control concepts to laboratory analyses requires that the analytical method itself be tested and validated periodically. Of course, this too will increase the average cost of a measurement, perhaps strain the resources of the laboratory, and add to the sample load. For many samples the investment in acquiring the sample and shipping it to the laboratory may be several hundred dollars. It does seem worthwhile to spend a few dollars per sample on analytical quality control (AQC). Nevertheless AQC is often deleted or reduced to a token level in the face cost and time pressures.

One solution to this dilemma is a real time computer system that acquires data from laboratory instruments, does all calculations including AQC statistics, and has the capability of exercising some measure of control over the

functioning of the instruments. Given such a system it should be possible to generally improve the overall quality of data, make realistic estimates of the uncertainty of measurements, and maintain reasonable costs and personnel workloads.

Table 1 includes some of the kinds of quality control measurements that are periodically made during a series of environmental measurements. EPA guidelines for environmental monitoring laboratories call for 10-20% of their effort to be devoted to quality control. The flow chart in Figure 1 shows the sequence of events that occur during a series of laboratory measurements with the EPA laboratory automation system. These events illustrate the interactive nature of the user-computer system, and explain the concept of real-time quality control. The example is taken from the Technicon AutoAnalyzer program.

The instrument operator starts the program and the program prints a series of prompts at the user's terminal that request information about the analysis to be performed. The operator responds to each question at the terminal keyboard. Inputs include an analysis title, operator name, date, sample numbers, standard concentrations, quality control pattern, and instrument operating parameters. The quality control pattern is the sequence of samples, check standards, duplicates, spikes, and blanks that will be run during the analysis. At the conclusion of the input, a sample holder pattern is printed to assist the operator in placing the appropriate sample, standard, etc. in the proper place in the automatic sample changer. The operator enters a one character command, and the analysis begins.

The first samples measured are standards to set the sample changer timing, blanks to measure the baseline, and concentration calibration standards. After these the environmental samples and quality control samples are measured. At the end of the first quality control pattern--which may typically include 5-30 environmental samples, a duplicate, a spike, and a check standard--another blank is read to adjust for baseline drift. Within seconds all computations are made, precision and accuracy are determined for the duplicates and spikes, and the precision and accuracy is compared with previously determined and stored values. The Shewhart and Cusum statistical methods are applied and a summary quality control report is presented at the terminal for the operator's inspection. If all is in control the analysis proceeds to the next batch of samples already placed in the sample holder. If out of control the operator is obliged to take appropriate action. The out of control samples will have to be rerun, but this information is known within seconds while the samples are still in the sample holder and not several hours or days later. If the system was in control and all samples were finished, the program prints an operator's report that includes a complete digest of the quality control information. If this is acceptable the operator orders, via a terminal command, a customer report printed. This also contains quality control information, but in a simpler and shorter format.

With the implementation of data management as described in another section, the sample numbers may optionally be entered into the user program from the backlog file. At the conclusion of the run, the operator will be asked if the results are approved for release to sample file control. If the

Table 1

Some Analytical Quality Control Procedures

Procedure	Application
Calibration Standard	Calibration standards are used to establish a relationship between a measured phenomena and concentration. Too few standards can lead to erroneous conclusions about the shape of the instrument response curve and inaccurate results.
Check Standard	The periodic measurement of a standard as an unknown is a check on instrument drift, reagent stability, and human errors.
Reagent Blank	A reagent blank contains all materials used in an analytical measurement except the sample. A periodic measurement of a blank is a check on baseline drift and background signals from reagent contamination.
Lab Duplicate	A periodic lab duplicate is revealing of errors due to instabilities in instruments, reagents, or analytes. Lab duplicates are used to establish the precision of the method as expressed by the standard deviation. A lab duplicate must include a repetition of the complete analytical procedure.
Field Duplicate	If the precision of the method is known, a periodic field duplicate can provide information about errors in sampling strategy or laboratory errors in record keeping and sample dilution.
Lab Spike	The periodic addition of a known amount of analyte to the sample can give information about changes in the analyte concentration due to settling, the presence of interferences, or improper preservation techniques.
Field Spike	Same as a lab spike except time begins in the field and effects that occur during shipment and storage are included.

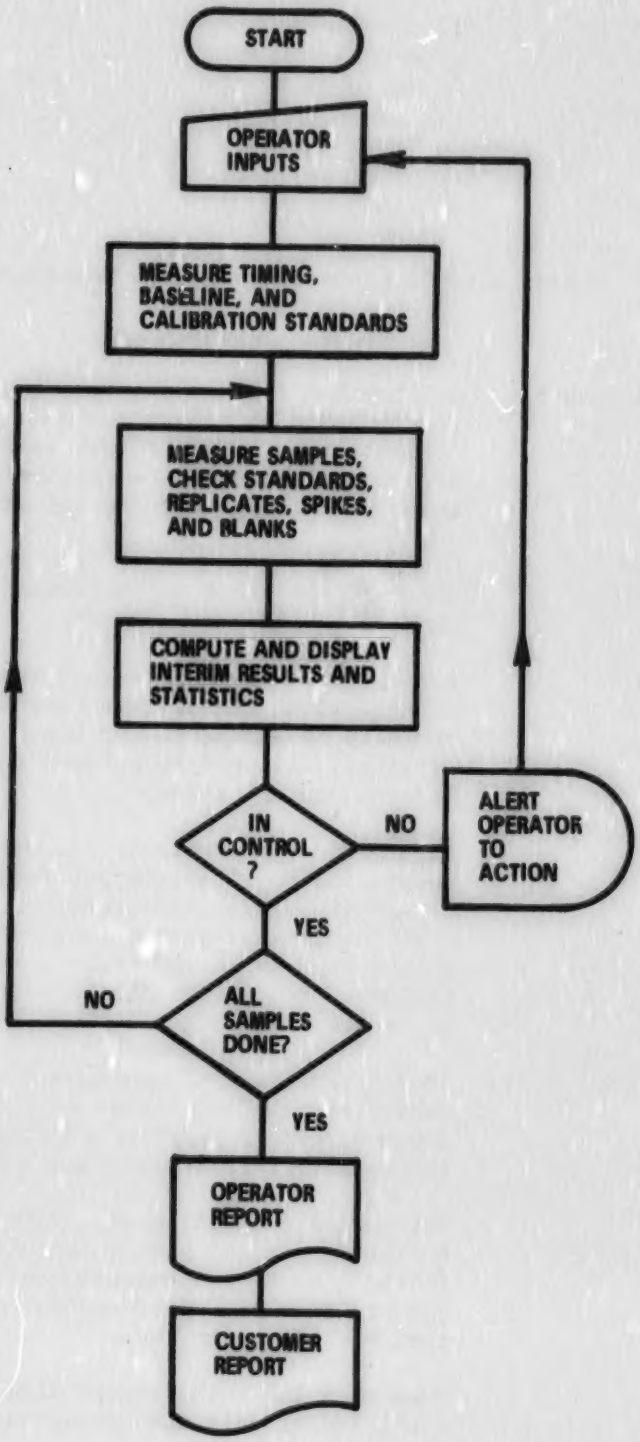

Figure 1. Flow Chart of the Sequence of Events During a Controlled Series of Laboratory Measurements.

operator and the laboratory management enter the release password, the environmental data and the quality control data will be transferred to the data management system. The printed unconsolidated report should be signed by the operator and retained as an extension of the laboratory notebook and a permanent legal record of the validity of the results.

There appears to be two distinctly different types of quality control derived from laboratory automation. One of these benefits is the ability to process in a cost-effective way the quality control procedures indicated in Table 1 and Figure 1. This quality control benefit is called active quality control because it still requires some action on the part of laboratory personnel to prepare the quality control samples. These additional samples are AQC overhead which is defined as the percentage of measurements made that do not generate environmental data, but either provide control information to the instrument operator or generate more realistic raw data for subsequent calculations. These measurements are of reagent blanks, duplicates, spikes, check standards, and calibration standards and all contribute to this overhead:

$$\text{AQC OVERHEAD} = \frac{\text{Sum of Blanks + Duplicates + Spikes + Standards}}{\text{Sum of All Measurements Made}} \times 100$$

The additional personnel effort required to process a 40% active quality control overhead is estimated to be about 1%. Additional instrument time is required to process this overhead. The principal personnel time savings is in the numerous calculations required to reduce the active quality control data to meaningful results.

A different kind of quality control benefit from laboratory automation is passive in the sense that no additional personnel effort is required to receive the benefit. It is purchased at the time of the original investment, it is present at all times, and it does not require an additional price each time it is used. Passive quality control is derived from the elimination of errors that result from hand measurements of peak heights or areas, the elimination of errors introduced by manual or desk calculator computations, and the elimination of errors that result during the transfer of data from one piece of paper to another piece of paper. Other errors eliminated are those that result from baseline drift and assumptions of linear calibrations when a non-linear equation is more accurate. Automation eliminates these problems since the computer automation system acquires all peak heights or areas, does all computations, corrects for baseline drift, calculates results based on the best mathematical fit of the calibration data, and prints a report that involves no hand copying of data.

SECTION IV

SUMMARIES OF WORK IN PROGRESS DURING FISCAL YEAR 1977

SYSTEMS INSTALLED AND FEASIBILITY STUDIES

Currently EPA has three instrument automation systems installed. All are based on the Data General model 840 minicomputer and use essentially the same software:

Environmental Monitoring and Support Laboratory-Cincinnati (EMSL-Ci)	Development and Test System
Cincinnati Computer Services and Systems Division (CSSD)	Cincinnati Environmental Research Center Production System (Supporting MERL)
Region V Surveillance and Analysis Laboratory	Production System and Regional Test Site

Studies are in progress to determine the feasibility of installing Data General based systems at several other sites. These studies are supported by the Management Information and Data Systems Division (MIDSD), and monitored by EMSL-Ci and CSSD. The status of these studies is as follows:

Region III Surveillance and Analysis Laboratory	submitted for approval
Region IV Surveillance and Analysis Laboratory	in progress
National Enforcement Investigation Center-Denver	in progress
Region VII Surveillance and Analysis Laboratory	in progress
Region II Surveillance and Analysis Laboratory	planned for FY '77
Open	planned for FY '77

SYSTEM SAMPLE PROCESSING CAPACITY

A number of benchmark tests of the capacity and quality control aspects of the EPA laboratory automation system are in progress. The Municipal Environmental Research Laboratory's Waste Identification and Analysis Section is one user of the Environmental Research Center's production system and recently reported some capacity data that was of interest. The section has interfaced four channels of Technicon AutoAnalyzer (TAA) and one flame atomic absorption (AA) spectrometer with a computer controlled sample changer. The maximum number of measurements per day was determined to be 200 for the AA spectrometer and 1600 for the four Technicon instruments. The Technicon equipment is broken down into a dual channel TAA I usually dedicated to nitrite and nitrite plus nitrate measurements, a single channel TAA II usually dedicated to phosphorus measurements, and a single channel TAA II usually dedicated to ammonia or total Kjeldahl nitrogen measurements. All have large sample changers holding 200 samples and the second production run of the day concludes about 10:30-11:00 PM unattended.

To estimate the number of measurements possible per year in this one laboratory it was assumed that maximum capacity runs would take place 50% of the available time and that all other available time would be utilized for preventive maintenance, operator continuing education, personnel sick leave, annual leave, and trouble shooting. The 50% capacity figures are as follows:

Instrument	Measurements/year
TAA I (2 channel)	104,000
TAA II	52,000
TAA II	52,000
AA	26,000
	234,000

Presently four additional channels of Technicon and two AAs are being interfaced to the computer system which is not yet at full instrument capacity.

ELECTRONIC BALANCE AUTOMATION

An electronic balance was interfaced to the laboratory automation system at the Region V laboratory, primarily for the purpose of weighing new and loaded air filters for particulate matter determinations. This balance is used for eight hours per day during certain periods and appears to be one of the most successful implementations of the system. Since there are many weighing operations involved in environmental laboratory operations, including National Pollution Discharge Elimination System (NPDES) measurements of filterable and non-filterable residues, it would appear reasonable to include an electronic balance in a laboratory automation system. For the information of those contemplating the purchase of an electronic balance, Region V has a Mettler model HE20 with a model BE20 balance control and a model BA28 digital readout. Interfacing these would be particularly cost-effective since the interface design and software already exist.

FLAMELESS ATOMIC ABSORPTION AUTOMATION

Recently the Perkin-Elmer model 503 atomic absorption spectrometer, which is interfaced to the EMSL-Ci development system, was fitted with a model HGA 2100 graphite furnace and a model AS-1 automatic sample changer. A new set of programs for application with the furnace and sample changer was developed and these are available at no cost to anyone who has the hardware to use them.

We believe this combination is a superb example of instrument automation. In one recent experiment 65 measurements of arsenic in the 2.5 - 100 µg/l range were accomplished in a little over three hours, including all calibration and quality control calculations. The 65 measurements included all standards and quality control samples. Actual operator intervention time was only about 30 minutes for sampler and program set-up and retrieval of the printed report. In our judgement the real advantage of these kinds of systems is the quality of output that can be sustained over an extended period of time.

DATA GENERAL AND DIGITAL EQUIPMENT MINICOMPUTERS

The Environmental Protection Agency signed a contract during 1976 with the Digital Equipment Corporation (DEC) for purchase of a number of PDP-11 model 45 and model 70 minicomputer systems. These minicomputer systems were intended for several applications including remote job entry to large Agency batch processing computers, relatively small mathematical models, and small regional databases. The terms of the DEC contract restrict direct customer hardware interfacing with a PDP-11. The Data General minicomputer was selected on the basis of quite different specifications including real time data acquisition and control capabilities. However, the top of the line PDP-11/70 will play a key role in laboratory automation according to current studies for the implementation of the Laboratory Data Management. The role of the PDP-11/70 in this area and the status of laboratory data management are discussed in Section VI of this report.

ULTRAVIOLET-VISIBLE SPECTROMETER AUTOMATION

For those contemplating a laboratory automation system, one instrument worth considering is a general purpose ultraviolet-visible spectrometer. At EMSL-CI we chose an existing moderately priced Perkin-Elmer (Coleman) model 124 spectrometer for addition to the development system. This instrument has about 1-2 nm resolving power and measurement accuracy sufficient for most general purpose work. The following application programs have been developed or are still under development, and all of these are available at no cost to anyone who has the hardware to use them:

1. NBS performance test (completed).

2. Data acquisition and reduction for the chlorophylls a, b, c and pheophytin a, and various chlorophyll and biomass ratios and indexes (completed - see later note in this section).

3. A color analysis system compatible with 304(g) requirements (under development).

4. A program for measurements of many NPDES analytes with manual sample preparation. These are analytes often measured with Technicon systems except when only a few samples are on hand or the samples require special treatment. All methods implemented will be approved 304(g) methods (under development).

EVALUATION OF TERMINALS

Keyboard/printers, keyboard/cathode ray tubes (CRT), and keyboard/CRT's with optional hard copy are the devices (terminals) used for communication between an instrument operator and a laboratory automation computer system. The selection of terminals for a system is one of the more perplexing aspects of the hardware design. The selection is a problem because there is a bewildering variety of terminals available and there needs to be a friendly relationship between an instrument operator and his terminal. Since not all operators are alike, a single terminal will not satisfy everyone. At EMSL-Ci we have deliberately chosen to acquire and evaluate user's responses to a variety of terminals. All terminals have a standard EIA plug and interface and can be easily interchanged. Also all operate at a minimum of 30 characters per second and therefore no ASR-33 teletypes are included. A list of terminals in use is as follows and we will be happy to share our experiences with anyone needing the information.

Terminal	Type	On EPA Standard Contract	Approximate Price ,($)	Speed char/sec
Lear-Siegler model ADM	CRT	No	1500	120
Digital Equipment model VT-52	CRT	Yes	2000	120
Texas Instruments model 700	Printer (heat sensitive paper)	Yes	1700	30
Hewlett-Packard model 2640B	CRT with memory for soft copy of about 8 screens	No	2900	120
Digital Equipment model VT-55	CRT with optional hard copy (slow & wet copy)	No	4000	120
Digital model LA-36	printer (ordinary paper)	No	1700	30
Tektronix model 4000 series	CRT with optional hard copy (fast copy)	Yes	7000 - 13,000	120

TRANSFER OF DATA FROM INSTRUMENTS WITH DEDICATED DATASYSTEMS

There are many laboratory instruments available that have built-in data processing capability in the form of microprocessors or even minicomputers. There is a general need to move data from these instruments to the laboratory automation system so that it may be further reduced and/or consolidated with other data for transfer to the sample file control system. Presently we have under design consideration a general solution to this problem based on a microprocessor controlled buffer concept.

A common feature within this class of instrumentation is the ability to output the raw or partly reduced data to an output device, usually a teletypewriter, in a standardized code (American Standard Code for Information Interchange, ASCII). Systems protocol inhibits the direct connection of the dedicated system's output port to the laboratory automation system's input port. However, if a microprocessor is placed between the two systems, the system protocol of the dedicated and lab automation systems can be maintained.

The microprocessor buffer will be hardwired to the output device of the dedicated system. This will allow the microprocessor to "catch" the ASCII characters and store the outputted report in a buffer area of the microprocessor's memory. The buffer system will then log into the laboratory automation system and transfer the ASCII data in its buffer memory to a disk file on the lab system via Basic language commands. This design concept should be applicable to many instrument types including:

1. Emission spectrometers with dedicated minicomputers.

2. GC/MS systems with dedicated minicomputers.

3. Gas chromatography data systems (small single purpose integrators or large multi instrument systems).

4. Other systems such as scintillation counters, x-ray spectrometers, etc.

GENERAL PURPOSE INTERFACE BUS (GPIB) AND EIA RS-232-C STANDARDS

The GPIB is a new Institute of Electrical and Electronics Engineers standard for a digital interface for programmable instrumentation (IEEE Standard 488-1975). The EIA RS-232-C is a widely used communications interface protocol. If you are in a position to purchase any new instrument, and the choices include one with a GPIB or EIA interface at moderate additional cost, e.g., a few hundred dollars, it is worth serious consideration to choose the GPIB or RS-232-C instrument if all other critical factors are equal. This will save considerable time and expense at some later date if that instrument is interfaced to a computer system.

POTENTIAL COST SAVINGS UNDERESTIMATED

The cost savings to the Agency that are possible with relatively standardized, but flexible, minicomputer systems are enormous. This is well

documented in the instrument automation system feasibility studies and the standard terminal procurement concept. One aspect of the cost savings that appears understated is the cost of acceptable software documentation. It appears in many cases that the cost of producing acceptable documentation may actually exceed the cost of writing the software. Thus standardized systems using similar general purpose software and the same documentation will accrue another cost saving. Acceptable documentation is defined as:

1. Step-by-step operational instructions covering all possible logical conditions, under both normal and most abnormal conditions.

2. System-level functional descriptions and operational flowcharts of all programs.

3. Up to date program listings and indexed magnetic tape copies of all programs with extensive commenting in the source code.

AUTOMATED CHLOROPHYLL ANALYSIS SYSTEM

The addition of the Perkin-Elmer (Coleman) model 124 ultraviolet-visible (UV-VIS) spectrometer to the EMSL-Ci pilot laboratory automation system makes possible the automation of several analytical methods used in the Environmental Protection Agency. The first method automated was the chlorophyll (Chl) analysis system and several benchmark tests were conducted to evaluate the productivity of the automated system. In this work five replicate absorption curves were obtained from an unacidified and an acidified aliquot of a 90% aqueous acetone pigment solution containing chlorophylls a, b, c and pheophytin a using the unautomated Beckman ACTA V spectrometer and the automated Perkin-Elmer 124. Records were maintained of the time required to carry out the scans and to calculate the concentrations of the pigments and biomass relationships in the sample. The mean, standard deviation and relative standard deviation were calculated for the following parameters: (1) Chl a, Chl b, Chl c and total chlorophyll (UNESCO trichromatic method); (2) Chl a/Chl b and Chl a/Chl c ratios; (3) (OD663 before acidification)/(OD665 after acidification); (4) Biomass (AFW)/Chl a (known as the autotrophic index); (5) Pheophytin a and corrected chlorophyll a (monochromatic method); (6) Revised total chlorophyll (using corrected chlorophyll a value); (7) Revised autotrophic index (using corrected chlorophyll a value); and (8) Revised Chl a/Chl b and Chl a/Chl c (using corrected chlorophyll a value).

The results obtained during the benchmark tests were as follows: (1) Samples were scanned with the ACTA V; absorption spectra were recorded on the strip chart recorder; all calculations were carried out manually on the Wang 320 desk calculator. The time required was 288 minutes, and (2) Samples were scanned on the automated Perkin-Elmer 124; all calculations were carried out on the laboratory computer. The time required was 43 minutes.

The mean chlorophyll a values obtained from the analysis of 5 replicate samples using the two instruments differed by less than 3%, and the relative standard deviation of the data obtained with the automated system was less

than 2%. We conclude that the saving in time and the expected quality assurance benefits from the automated system are very significant and fully justify the cost of the development work. Additional benchmarks are planned to further evaluate the system with respect to the precision and accuracy of the measurements.

SECTION V

AN OVERVIEW OF THE HARDWARE AND SOFTWARE OPERATIONS OF THE INSTRUMENT AUTOMATION SYSTEM

The EPA instrument automation system uses commercial computer hardware and software. Extensions to the hardware and software were developed during the project to complete the instrument automation. Flexibility and adaptability in automating similar laboratories was incorporated into the basic system design.

The Computer

The heart of the instrument automation system is a Data General Corporation model 840 Nova Computer or any compatible computer that uses the same instruction set. Multiply-divide and floating point hardware are included to enhance processing speed. A hardware memory mapping and protection unit is used to allow two programming grounds to operate independently and hardware protected from each other. The sixteen bit processor is equipped with 64K of core memory. This allows 31K of memory for the instrument operators' multiuser Basic language programs executing in the foreground, and approximately 18K of memory for utility programs executing in the background. The remaining 15K of memory is dedicated to the Mapped Real Time Disk Operating System (MRDOS).

The mass storage devices are a high speed fixed head disk for system overlays and swapping files, a slower moving head disk for fast access to program and data files, and a 9 track magnetic tape for system dumps, off-line storage, and interlaboratory distribution of programs. A medium speed line printer is available for outputting final reports and program listings.

Figure 2 is a block diagram of the current EMSL-Ci pilot development system. Figure 3 is a block diagram of the CSSD system that currently supports the Municipal Environmental Research Laboratory (MERL). The Region V system has an essentially identical computer configuration, but a slightly different mix of instruments.

User communication with the automation system is accomplished with any type of terminal, i.e., printer or cathode ray tube (CRT) that has a standard EIA RS-232-C interface. The foreground and background terminals are used for system type operations, while the instrument operators execute applications programs from terminals at the instrument sites. Since the system is a multiuser system, all users appear to have simultaneous access to the Basic language capabilities through the terminal multiplexer.

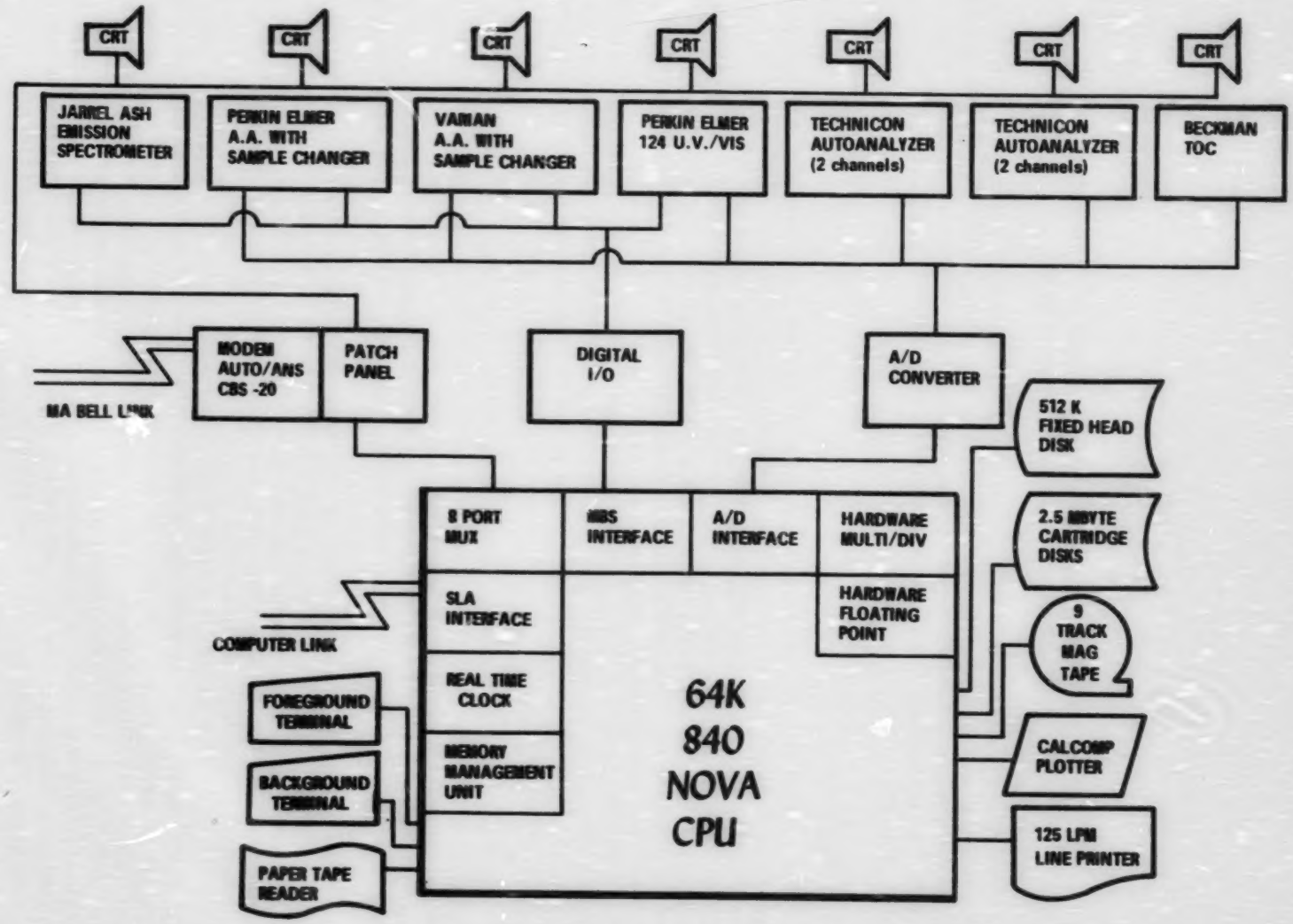

Figure 2. A Block Diagram or the EMSL-Cincinnati Pilot Laboratory Automation System

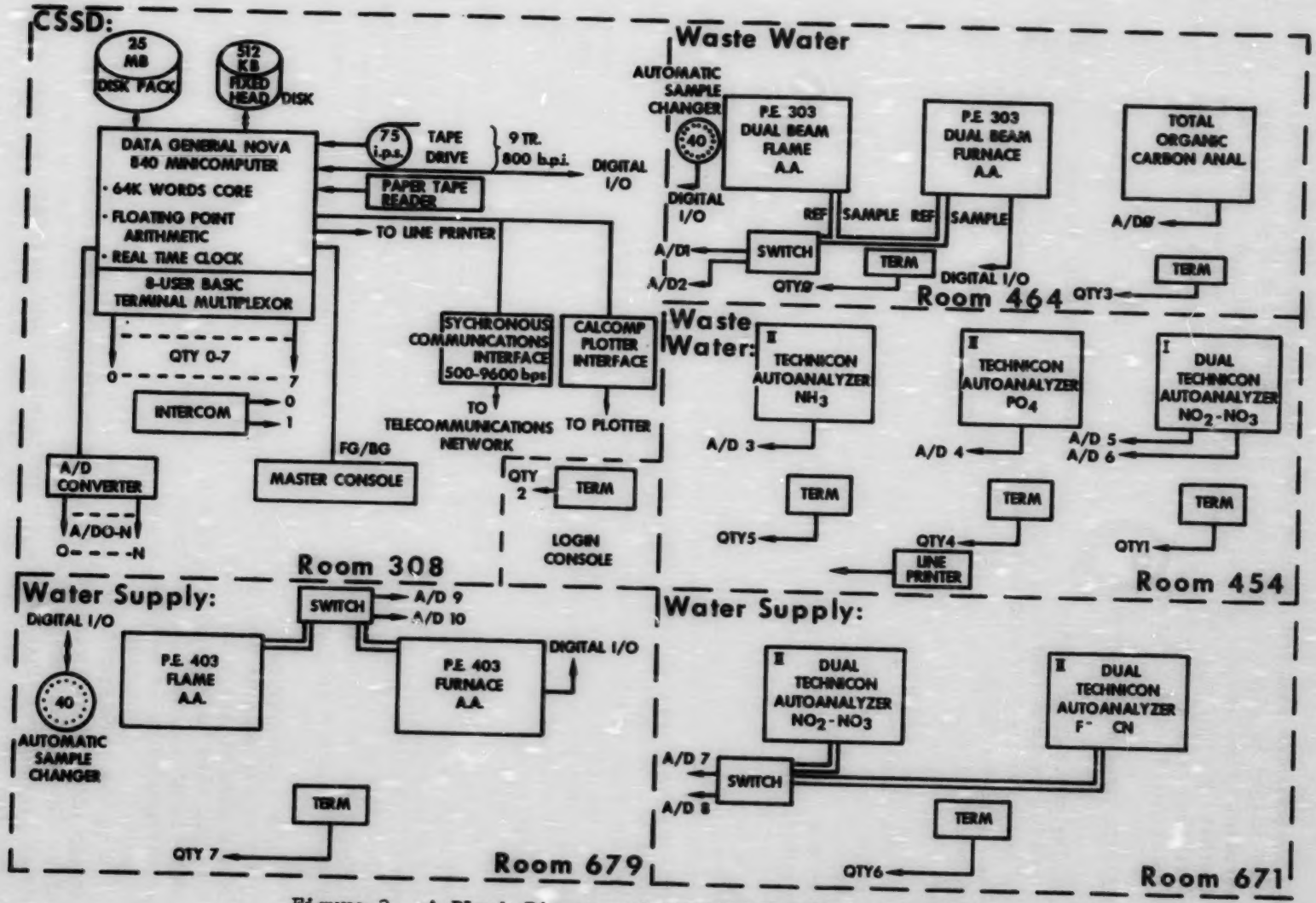

Figure 3. A Block Diagram of the CSSD Production System.

Instruments that generate analog signals are interfaced through a multiplexed analog to digital converter. Instruments with digital output or instruments that are controlled with digital signals are interfaced through a commercially available (MDB Systems) digital interface card. A more complete description of the computer and interface hardware is in preparation and will be published in a future report.

OPERATING SYSTEM AND SOFTWARE

The overall operation of the laboratory instrument automation system is controlled by Data General's mapped real-time disk operating system (MRDOS). This occupies about 15,000 words of core memory with overlays of the high speed fixed head disk. The MRDOS handles all input and output from the standard peripherals (disks, tapes, printer, etc.) and controls priorities among the various tasks running in the system.

The high level interpreter language, extended Dartmouth Basic, is used for the instrument data acquisition, data reduction, and data report applications (user) programs. This powerful but easy to learn language was specified for the user applications programs in order to assure that control of computational methods and report formats would reside with the laboratory science professionals. Basic has powerful computational capabilities, yet it is very easy to learn and is widely taught in high schools and colleges. It does not require detailed knowledge of computer systems and hardware, and a professional programmer is not required for day to day laboratory operations. The inevitable and frequent small program changes may be made in seconds by laboratory personnel from the instrument terminals. The Basic language was the only high level language, available on a mini-computer that permitted some users to run data acquisition programs while other users, simultaneously, modified existing programs or wrote new applications programs. This same level of flexibility allows the convenient addition of additional applications programs to the system.

The Basic language is somewhat less efficient in its use of computer resources (memory, etc.) and it runs slower than a compiled language (Fortran) or a machine language program. However, the advantages of Basic in increasing overall laboratory personnel productivity far outweigh its disadvantages. The execution speed of Data General's extended Basic is sufficient to allow rapid response times at the user terminals. The vast majority of laboratory instruments have a sufficiently slow data rate and pose no serious problem.

The multiuser Basic language interpreter and all user programs run in 31,000 words of core memory called foreground. The remaining core memory is assigned to the background. Foreground programs always have a higher priority than background programs and input from instruments has the highest priority of all tasks. Background programs run during intervals of time when no foreground tasks require attention.

In the foreground, the Basic language interpreter and its extensions occupy about 17,000 words of core memory with overlays on the high speed disk. The extensions to Basic include a series of machine (assembly) language subroutines that handle the critically timed acquisition of data from

instruments and the digital control functions. Applications programs for each instrument in the Basic language make calls to the machine language subroutines whenever data points are acquired from an instrument or a control function is executed.

The Basic language applications programs vary in size and are stored on the cartridge disk. When a user runs a program it is loaded into the remaining 13,000 words of foreground user memory. Several users may run programs simultaneously, and as long as this memory is adequate, all user programs are core resident. As soon as the combined size of the user programs exceeds the 13,000 words of memory, swapping to the high speed fixed head disk begins. Each user program is allocated a few milliseconds of run time, and then the program is written to the swapping disk. At the end of another few milliseconds the user program is returned to core memory for another brief period of run time. This round robin swapping continues for as long as the combined requirements of the users programs exceeds the 13,000 words of foreground core memory. While the user program is swapped out of core memory, no instrument data is lost because the machine language data acquisition and control subroutines are always core resident. The instrument user is generally unaware of swapping as it is too fast to be noticeable.

LABORATORY INSTRUMENTS

The complement of instruments at each laboratory automation site was intended to be flexible and allow for easy addition of new instrumentation. Figures 2 and 3 show the current Cincinnati complements, and Table 2 gives more information about these and the Region V system. Table 2 also lists the maximum supported number of each type of instrument in a given system. The maximum number of concurrent users is not exactly established, but probably is in the range of 12-16. For each instrument implemented, one or more applications programs have been developed, tested, and largely debugged.

It should be noted that in a few selected applications of analytical instrumentation, manufacturers have found it either necessary or profitable to develop mini-computer systems dedicated to very specific instruments. These applications include:

* Gas chromatography with conventional detectors
* Gas chromatography-mass spectrometry
* Nuclear magnetic resonance
* X-ray analysis
* Radiochemical analysis

The manufacturer's development costs (many millions in some cases) for these are spread among the large number of units sold. Therefore, it was more cost effective and technically feasible to use the commercial "stand alone" systems than to interface the respective instruments to the laboratory automation system. However, the laboratory automation system was designed

Table 2

Maximum Supported Number of Laboratory Instruments of Each Type on the EPA Laboratory Automation System

Types of Instruments	Maximum Supported Number of Each	Location Where at Least One is Implemented
Technicon AutoAnalyzer I (single, dual, triple, and 6 channel)	12 channels	MERL
Technicon AutoAnalyzer II (single, dual, triple, and 6 channel)	12-n channels (n = the number of TAA I channels)	Region V EMSL-Ci MERL
Partial Control for Technicon Sample Changers	8	None
Perkin-Elmer, Instrumentation Lab, etc. double beam flame atomic absorption (AA) spectrometers	4	Region V EMSL-Ci MERL
Varian single beam flame atomic absorption spectrometers	4	EMSL-Ci
Lawrence Livermore Laboratory Computer driven Sample Changers for flame atomic absorption spectrometers	8	Region V EMSL-Ci MERL
All types of flameless high temperature furnace atomic absorption spectrometers	4	Region V EMSL-Ci MERL
Partial control for Perkin-Elmer flameless AA high temperature furnace sample changers	4	EMSL-Ci
Jarrel-Ash Analog or Digital Interfaced Emission Spectrometer	1	EMSL-Ci
Ultraviolet-Visible, Infrared, etc. wavelength scanning spectrometers	2	EMSL-Ci
Beckman type total organic carbon analyzers	2	EMSL-Ci MERL
Partial Control for total organic carbon sample changers	2	None
Electronic Balances	2	Region V
Instruments with dedicated mini-computer or micro-processors	8	None

for versatility, and plans for interfacing these systems were described in Section IV of this report. This will allow an expansion of the capabilities of the dedicated computers and permit output of comprehensive reports.

All instrument hardware interface designs are in the public domain and are documented in the engineering drawings and parts lists. These interfaces may be readily reproduced on contract to organizations that specialize in the manufacture of printed circuit board modules.

SECTION VI

OVERALL PLAN FOR THE INTEGRATION OF INSTRUMENT AUTOMATION AND LABORATORY DATA MANAGEMENT SYSTEMS

For the last three years there has been a great deal of discussion and study of a management information system for EPA laboratories. The major factor that has impeded the development of this system has been the failure to develop a set of sufficiently clear and detailed written functional specifications that are broadly acceptable within the Agency. A new set of specifications is now available which integrated previous studies and added much new information. If there is sufficient concurrence with the Agency, a system based on these specifications could be implemented within the next year.

In the meantime, several hardware environments have been considered for the implementation of the laboratory data management capability:

(1) One of the large Agency-wide batch/time sharing computer systems. The Data General instrument automation system and the large computer system would communicate by remote job entry emulator software operating in the background of the Data General minicomputer. The system would be supported by laboratory and/or program (regional) office data processing staffs.

(2) The background of the Data General instrument automation computer with support by the laboratory staff.

(3) A second Data General computer in the laboratory with communication to the instrument system through a shared disk memory. The system would be supported by the laboratory staff.

(4) A (regional) program office PDP-11/70 computer. The Data General instrument automation system and the PDP-11/70 would communicate by remote job entry emulator software and the system would be supported by laboratory and office data processing staffs.

After a lengthy period of study, including benchmark testing of several alternatives, all but option 4 have been eliminated as viable implementation possibilities. Option (1) was eliminated because of the slow turnaround and high costs of the large Agency systems. Option (2) was eliminated because the single Data General system does not have the capability to concurrently and reliably process instrument inputs and laboratory data management. Option (3) was eliminated because of the unavailability of appropriate software and utilities for laboratory data management. The INFOS software package and other general purpose software offered by Data General was judged to

require a great deal of additional development in order to be applicable to the EPA laboratory data management system. Also there was a general lack of capability to maintain data management type software in the EPA laboratories.

Option (4) was considered especially attractive because of the Agency decision to adopt Digital Equipment Corporation PDP-11 computers for decentralized processing. This choice for laboratory data management would provide functional independence of instrument automation and data management systems. Reliability would be enhanced in the sense that hardware or software malfunctions in one system would not affect the other system. Also program or regional office data processing staffs have the general capability to support data management software, and it would be easier to support if it were integrated into the single data management package planned for EPA office minicomputers. This alternative is also consistent with the fact that more laboratories may require laboratory data management than instrument automation. Therefore, many laboratories would not have access to an instrumentation computer for data management, but could use the program office system directly for this purpose.

Figure 4 shows a block diagram of a hierarchical distributed computer system that includes on-line laboratory data acquisition, laboratory data management, and links to large Agency batch processing computers with access to national databases. The hierarchical network is the basis for current planning of integrated instrument automation and laboratory data management systems.

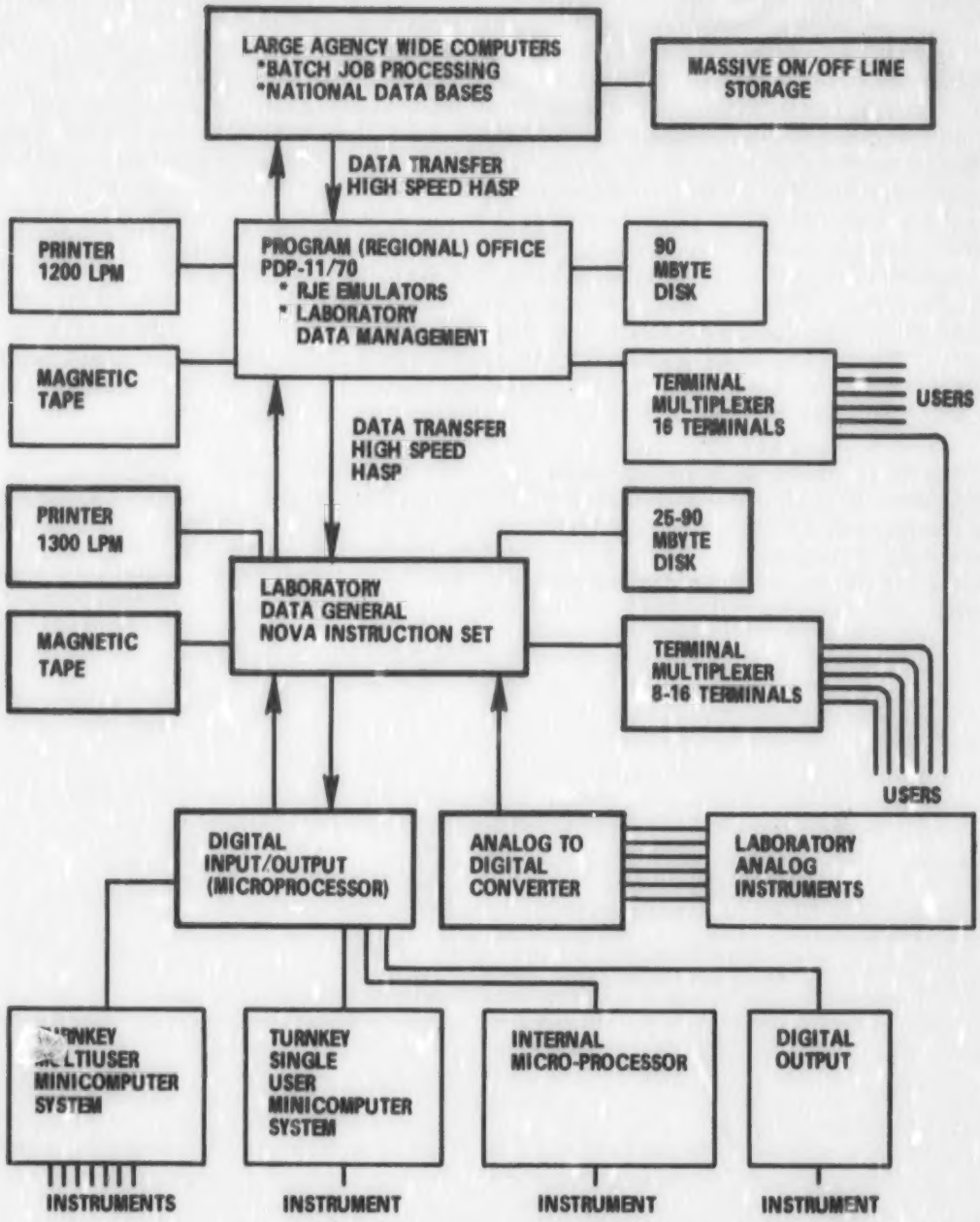

Figure 4. Hierarchial Computer Network for On-Line Laboratory Data Acquisition Data Management.

SECTION VII

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